Structural Formation of Huntingtin Exon 1 Aggregates Probed by Small-Angle Neutron Scattering

Christopher B. Stanley,† Tatiana Perevozchikova,‡ and Valerie Berthelier‡

†Neutron Scattering Science Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831
‡Graduate School of Medicine, University of Tennessee Health Science Center, 1924 Alcoa Highway, Knoxville, TN 37920

Supporting Material

To calculate the cross-sectional radius of gyration for the three hollow cylinder models representing 1, 2, and 3 filaments of the Perutz β-helix model in Fig. 4D, we derived Eqs. 7a, 7b, and 7c from the mass moment of inertia and parallel axis theorem.

I. Derivation of Eq. 7a

For the single hollow cylinder cross-section shown in Fig. 4D.1 with inner radius, R_i, and outer radius, R_o, the mass per length

$$m = \pi\rho\left(R_o^2 - R_i^2\right)$$

where ρ = density. The mass moment of inertia of this single hollow cylinder cross-section

$$\begin{aligned} I &= \int_0^{2\pi}\int_{R_i}^{R_o} \rho r r^2 dr d\theta \\ &= 2\pi\rho\int_{R_i}^{R_o} r^3 dr \\ &= \frac{1}{2}\pi\rho\left(R_o^4 - R_i^4\right) \\ &= \frac{1}{2}\pi\rho\left(R_o^2 - R_i^2\right)\left(R_o^2 + R_i^2\right) \\ &= \frac{1}{2}m\left(R_o^2 + R_i^2\right) \end{aligned}$$

The cross-sectional radius of gyration

$$R_c = \sqrt{\frac{I}{m}}$$

yielding the single hollow cylinder cross-sectional radius of gyration

$$R_{\text{c,f1}} = \left(\frac{R_{\text{i}}^2 + R_{\text{o}}^2}{2}\right)^{1/2}$$

II. Derivation of Eq. 7b

Using the parallel axis theorem

$$I = I_i + md^2$$

where I_{i} = mass moment of inertia from the origin and d = displacement from the origin, the two and three hollow cylinder cases were derived. As shown in Fig. 4D.2 for the cross-section of two adjacent hollow cylinders each with $d = R_o$ from the axis of rotation

$$R_{\text{c,f2}} = \left(\frac{2\left(I_{\text{i}} + md^2\right)}{m}\right)^{1/2}$$

$$= \left(\frac{2\left(\frac{1}{2}m\left(R_o^2 + R_i^2\right) + mR_o^2\right)}{m}\right)^{1/2}$$

$$= \left(R_{\text{i}}^2 + 3R_{\text{o}}^2\right)^{1/2}$$

III. Derivation of Eq. 7c

As shown in Fig. 4D.3 for the cross-section of three hollow cylinders each with $d = (\sqrt{3}/2)R_o$ from the axis of rotation

$$R_{\text{c,f3}} = \left(\frac{3\left(I_{\text{i}} + md^2\right)}{m}\right)^{1/2}$$

$$= \left(\frac{3\left(\frac{1}{2}m\left(R_o^2 + R_i^2\right) + m\left(\frac{\sqrt{3}}{2}R_o\right)^2\right)}{m}\right)^{1/2}$$

$$= \left(\frac{3}{2}R_{\text{i}}^2 + \frac{15}{4}R_{\text{o}}^2\right)^{1/2}$$